Designing Better Microelectronics Devices

THE Laboratory, with its benchmark atomic-level materials theory and simulation software, has much to offer private industry in the area of microelectronics research. Only a few years ago, the idea of building a microelectronics device on an atom-by-atom basis might have seemed unrealistic. Now, that idea is within reach.

In May of last year, LLNL announced a cooperative research and development agreement (CRADA) with the Wilson Center for Research and Technology of Xerox Corporation, located near Rochester, N.Y. The three-year, $3-million project will investigate the behavior of individual atoms and molecules on the surface of micro-electronic materials, such as those used in semiconductor chips. The goal is to develop a fundamental scientific knowledge of surface processes, leading to improved performance of devices used in a variety of industrial and consumer electronics products. (For more information about Laboratory research on surface processes, see the article on p. 25.)

The joint research applies quantum mechanical principles to understand what happens when a few atoms interact with a surface. That understanding is expanded to include interactions of larger numbers of atoms, then layers of atoms, and, eventually, to quantities large enough to build entire microchips. The outcome of this approach could optimize, and possibly revolutionize, the processes by which new materials and devices are made.

At Xerox, researchers shine a beam of atoms at a surface and study the results, but they need a better theoretical base to interpret what they observe. The Laboratory's expertise in computer modeling can extend the state-of-the-art capabilities at Xerox in surface etching, passivating chemically reactive surface sites, and thin-film growth. For the Laboratory, the new experimental work will be invaluable in refining new models and validating theories.

Among other benefits, the collaboration may lead to an improved theory of reactive scattering—the scattering of atoms and molecules off semiconductor surfaces. Such a theory would allow scientists to predict the behavior of etching species that come into contact with a surface and cause a chemical reaction between two materials.

To develop a quantitative theory of reactive scattering, Laboratory scientists are calculating from first principles the electronic structure of chlorine atoms on a tantalum surface. Simulating all the dynamics from first principles is beyond the current capabilities of our best supercomputers. To circumvent this problem and address the industrial process of reactive etching, Laboratory scientists are using the first-principles energy of a single chlorine atom as it reacts with the tantalum surface; from this energy, we can set the parameters of an empirical potential energy model. Forces in classical molecular dynamics simulations are represented using empirical potential models (see the article on p. 13). Classical molecular dynamics is then used to model the industrial process.

By predicting and controlling these and other types of reactions, microelectronics devices could be built one atom at a time. Down the road, this would mean higher-density and higher-performance optoelectronic and microelectronic circuitry, larger-area displays, and advanced chip designs. For now, the work is considered "precompetitive research," meaning that the results will be made available to the scientific community with the expectation of commercial benefits in the future.

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